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SUPPLEMENTARY MATERIAL TO

ADMET profiles of selected anabolic steroid derivatives

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Table S-I. Fulfilment, by the investigated steroids, of the rules revealing oral bioavailability (Lipinski) and safety (Pfizer and GSK)

Steoid	Lipinski rule	Pfizer rule
methasterone	+	-
methyl-1-testosterone	+	-
4-hydroxytestosterone	+	+
methyldienolone	+	+
methyltrienolone	+	+
19-nor-5-androstenedione	+	+
oxymetholone	+	+

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Table S-II. ADMETLab2.0 prediction of the probability that the investigated steroid derivatives are substrates/inhibitors of human cytochromes (CYPs) involved in xenobiotic metabolism.

Steroid name / cytochrome	substrate					inhibitor				
	CYP1A2	CYP2C19	CYP2C9	CYP2D6	CYP3A4	CYP1A2	CYP2C19	CYP2C9	CYP2D6	CYP3A4
methasterone	0.666	0.951	0.308	0.866	0.641	0.066	0.092	0.263	0.012	0.309
methyl-1-testosterone	0.561	0.923	0.180	0.471	0.869	0.060	0.415	0.249	0.095	0.740
4-hydroxy testosterone	0.585	0.732	0.161	0.845	0.269	0.105	0.085	0.240	0.013	0.056
Methyl dienolone	0.528	0.458	0.149	0.125	0.707	0.143	0.088	0.230	0.492	0.323
Methyl trienolone	0.404	0.730	0.161	0.066	0.726	0.229	0.165	0.210	0.572	0.844
19-nor-5-androstenedione	0.705	0.749	0.803	0.884	0.628	0.087	0.170	0.339	0.007	0.237
oxymtholone	0.665	0.891	0.164	0.617	0.598	0.024	0.045	0.175	0.014	0.439

Table S-III. admetSAR2.0 prediction of the probability that the investigated steroid derivatives to be substrates/inhibitors of the human cytochromes (CYP) involved in metabolism of xenobiotics.

Steroid name / cytochrome	substrate			inhibitor				
	CYP2C9s	CYP2D6s	CYP3A4s	CYP1A2i	CYP2C19i	CYP2C9i	CYP2D6i	CYP3A4i
methasterone	-0.827	-0.803	0.689	-0.500	-0.872	-0.690	-0.973	-0.858
methyl-1-testosterone	-1.000	-0.880	0.677	-0.598	-0.766	-0.810	-0.969	-0.844
4-hydroxy testosterone	-0.728	-0.852	0.751	-0.893	-0.860	-0.928	-0.936	-0.881
Methyl dienolone	-0.828	-0.892	0.686	-0.900	-0.666	-0.950	-0.945	-0.881
Methyl trienolone	-1.000	-0.900	0.671	-0.900	-0.666	-0.950	-0.945	-0.881
19-nor-5-androstenedione	-0.788	-0.788	0.544	-0.826	-0.790	-0.927	-0.940	-0.865
oxymetholone	-1.000	-0.871	0.688	-0.838	-0.863	-0.857	-0.964	-0.806

Table S-IV. Predicted values for the probabilities of the investigated steroids to produce toxicological effects

Steroid name/prediction tool	ADMETLab2.0				admetSAR2.0			
toxicity	Carc.	Ames mut.	Eye corr.	Eye irr.	Carc.	Ames mut.	Eye corr.	Eye irr.
methasterone	0.062	0.039	0.003	0.016	-0.900	-0.980	-0.988	-0.941
methyl-1-testosterone	0.499	0.011	0.004	0.021	-0.900	-0.910	-0.991	-0.978
4-hydroxytestosterone	0.058	0.049	0.003	0.012	-1.000	-0.830	-0.994	-0.939
methyldienolone	0.634	0.031	0.003	0.014	-0.971	-0.910	-0.994	-0.932
methyltrienolone	0.881	0.016	0.003	0.014	-0.914	-0.780	-0.994	-0.974
19-nor-5-androstenedione	0.874	0.017	0.003	0.031	-0.900	-0.930	-0.987	-0.920
oxymetholone	0.129	0.013	0.004	0.017	-0.970	-0.960	-0.995	-0.996

Carc. – Carcinogenicity: Ames mut. - Ames mutagenesis, Eye corr. - Eye corrosion; Eye irr. - Eye irritation

Table S-V. Predicted values for the probabilities of the investigated steroids to bind to nuclear receptors (NR): AR – androgen receptor, LBD – ligand binding domain, AhR – aryl hydrocarbon receptor, ER – estrogen receptor, PPAR gamma – peroxisome proliferator-activated receptor gamma.

Steroid name / effect on the nuclear receptors	NR-AR	NR-AR-LBD	NR-AhR	NR-ER	NR-ER-LBD	NR-PPAR-gamma
methasterone	0.092	0.239	0.001	0.323	0.833	0.015
methyl-1-testosterone	0.079	0.743	0.000	0.182	0.850	0.022
4-hydroxytestosterone	0.061	0.025	0.000	0.186	0.816	0.158
methyldienolone	0.766	0.940	0.058	0.619	0.735	0.633
methyltrienolone	0.843	0.979	0.064	0.739	0.821	0.871
19-nor-5-androstenedione	0.710	0.793	0.033	0.87	0.844	0.667
oxymetholone	0.459	0.691	0.001	0.119	0.553	0.732

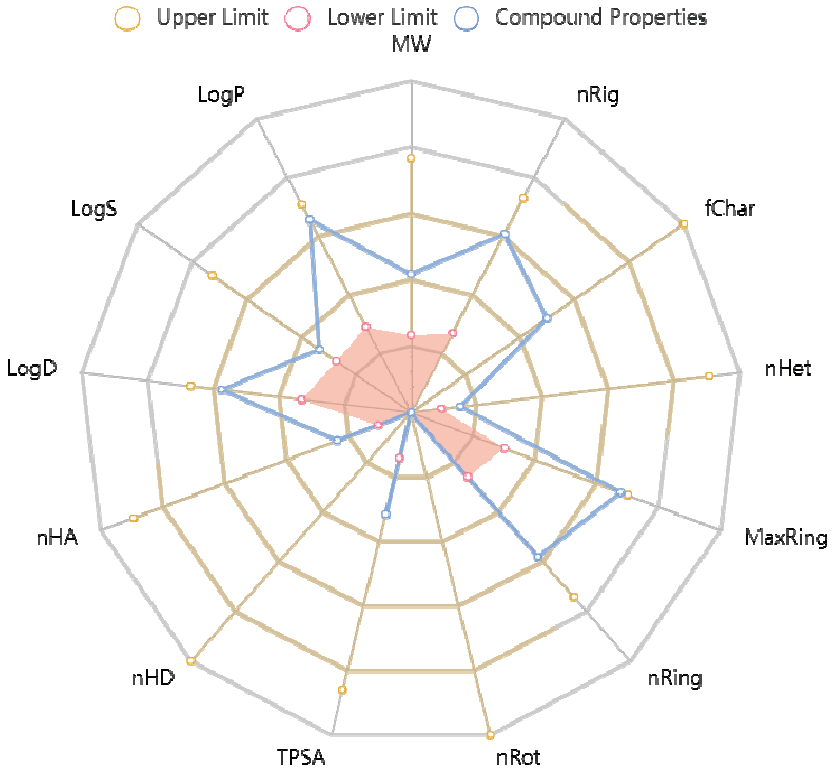

Figure S-1. The distribution of the properties of 19-nor-5-androstenedione (blue line) compared to the properties considered by the prediction models (yellow zone).